



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:12 PM UTC

PDB ID : 3ZZU / pdb_00003zzu
Title : Crystal structure of Staphylococcus aureus elongation factor G with mutations M16I and F88L
Authors : Koripella, R.K.; Chen, Y.; Selmer, M.; Sanyal, S.
Deposited on : 2011-09-05
Resolution : 2.98 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

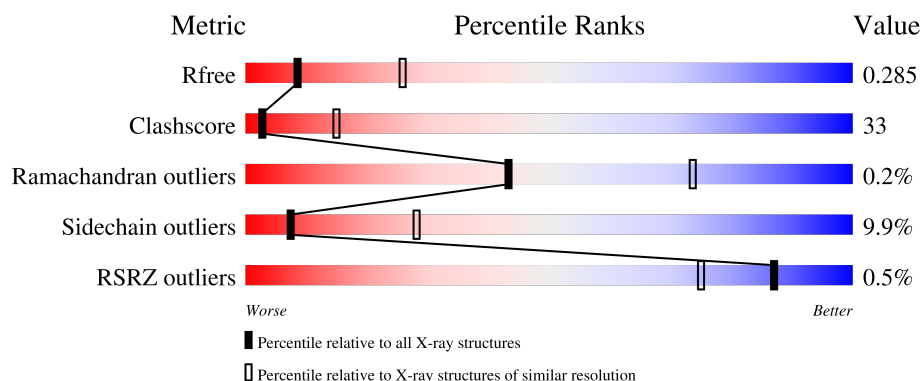
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

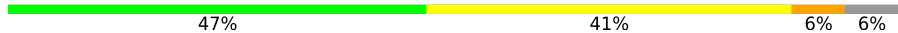
The reported resolution of this entry is 2.98 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3580 (3.00-2.96)
Clashscore	190562	3904 (3.00-2.96)
Ramachandran outliers	187476	3761 (3.00-2.96)
Sidechain outliers	187428	3764 (3.00-2.96)
RSRZ outliers	180081	3579 (3.00-2.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	693	
1	B	693	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10039 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called ELONGATION FACTOR G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	649	Total	C	N	O	S	0	0	1
			5018	3151	841	1000	26			
1	B	649	Total	C	N	O	S	0	0	1
			5018	3151	841	1000	26			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	16	ILE	MET	engineered mutation	UNP P68790
A	88	LEU	PHE	engineered mutation	UNP P68790
B	16	ILE	MET	engineered mutation	UNP P68790
B	88	LEU	PHE	engineered mutation	UNP P68790

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	O	0	0
			2	2		
2	B	1	Total	O	0	0
			1	1		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: ELONGATION FACTOR G



• Molecule 1: ELONGATION FACTOR G



P635	P636	G637	Q640	V641	V646	P647	L648	S649	E650	M651	L658	R659	S660	N661	T662	Q663	T667	M670	Y671	Y675	A676	E677	V678	I682	A683	I686	I687	K688	K689	M690	K691	G692	GLU																				
P558	L559	K563	A564	K565	D568	G569	S570	Y571	H572	D573	V574	D575	M579	A580	F581	K582	K590	A593	C596	D597	P598	V599	I600	M605	K606	V607	E610	M611	P612	E613	E614	Y615	M616	G617	D618	I619	M620	G621	D622	V623	T624	S625	R626	R627	G628	R629	V630	D631	G632	M633	E634		
C473	N474	V475	G476	A477	R483	E484	K487	S488	F496	S497	ARG	GLN	SER	GLY	GLY	ARG	Q505	H510	E511	E512	N516	E517	E523	E524	E525	N526	A527	I528	V532	V533	P534	R535	E536	Y537	I538	P539	S540	L545	K546	D547	A548	M549	E550	V553	L554	A555	G556	Y557					
S400	MET	GLU	PHE	P404	E405	P406	L410	S411	V412	E413	P414	K415	D419	Q420	D421	K422	Q425	K429	Q431	E432	E433	D434	P435	T436	H440	T441	D442	GLU	THR	GLY	Q447	V448	I449	L450	G451	G452	M453	L456	H457	L458	D459	R464	M465	K466	K467	E468	F469	N470	V471	E472			
V316	E233	E234	I235	S236	V237	S238	E239	L240	K241	I244	S245	Q246	A247	N250	V251	E252	F253	V256	L257	T260	K263	N264	K265	L269	M270	L271	D276	Y277	L278	P279	S280	P281	I287	T288	G289	H290	R291	A292	S293	V299	I300	A301	K302	A303	D304	E308	F309	L312					
V318	T318	D319	P320	V321	V322	F328	V330	G333	T334	K335	S337	Y340	V341	K342	N343	K346	G347	K348	R349	E350	K351	V352	G353	R354	L355	K363	Q364	E365	I366	V369	Y370	S371	G372	D373	I374	D382	L389	C390	G391	E392	A393	N394	D395	I396	L397	L398	E399						
R154	L155	Q156	I162	Q163	L164	P165	A168	E169	D170	E171	F172	E173	A174	I175	I176	D177	L178	V179	E180	M181	K182	C183	F184	Y186	T187	G191	T192	E193	E196	I199	P200	E201	D202	A210	R211	L214	I215	E216	A217	V218	A219	S222	D223	E224	L225	M226	E227	K228	Y229	L230			
I79	P83	G84	H85	V86	D87	L88	T89	V90	E91	V92	E93	R94	G101	A102	V103	Q109	S110	G111	V112	E113	F114	Q115	T118	V119	W120	R121	Q122	A123	T124	T125	Y126	G127	V128	R130	I131	V132	F133	V134	N135	K136	M137	D138	K139	N143	F144	E145	Y146	S147	T150	L151			
MET	A2	R3	E4	F5	S6	L7	E8	K9	A17	H18	I19	K23	R29	I30	L31	Y32	Y33	T34	G35	R36	ILE	HIS	LYS	ILE	GLY	GLU	THR	HIS	GLU	GLY	ALA	SER	GLN	MET	ASP	TRP	MET	GLU	GLN	GLN	ASP	ARG	GLY	ILE	THR	ILE	THR	S65	T68	T69	A70	H75	R76

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	65.20Å 125.52Å 106.90Å 90.00° 108.21° 90.00°	Depositor
Resolution (Å)	47.15 – 2.98 47.15 – 2.98	Depositor EDS
% Data completeness (in resolution range)	93.3 (47.15-2.98) 93.3 (47.15-2.98)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 2.96Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.237 , 0.294 0.232 , 0.285	Depositor DCC
R_{free} test set	1483 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å ²)	94.5	Xtriage
Anisotropy	0.135	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 105.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.035 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10039	wwPDB-VP
Average B, all atoms (Å ²)	115.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.95% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.37	1/5103 (0.0%)	0.81	4/6901 (0.1%)
1	B	0.35	1/5103 (0.0%)	0.83	10/6901 (0.1%)
All	All	0.36	2/10206 (0.0%)	0.82	14/13802 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	691	LYS	C-N	-6.98	1.23	1.33
1	B	691	LYS	C-N	-6.86	1.23	1.33

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	634	GLU	CA-C-N	-8.06	112.15	120.85
1	B	634	GLU	C-N-CA	-8.06	112.15	120.85
1	A	621	GLY	N-CA-C	-6.19	106.07	113.99
1	B	537	TYR	N-CA-C	5.71	120.25	113.28
1	B	632	GLY	N-CA-C	5.36	118.57	110.75
1	A	416	SER	CB-CA-C	-5.31	109.47	115.79
1	A	162	ILE	N-CA-C	-5.21	107.67	112.83
1	A	215	ILE	N-CA-C	5.20	117.58	111.09
1	B	277	TYR	N-CA-C	5.15	119.66	113.17
1	B	405	GLU	CA-C-N	5.08	126.20	119.84
1	B	405	GLU	C-N-CA	5.08	126.20	119.84
1	B	448	VAL	N-CA-C	5.06	116.53	109.80
1	B	156	GLN	N-CA-C	-5.04	106.71	112.86
1	B	613	GLU	N-CA-C	5.00	117.12	111.11

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5018	0	4936	330	0
1	B	5018	0	4936	330	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
All	All	10039	0	9872	658	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 33.

All (658) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:610:GLU:OE2	1:B:636:ARG:NH1	1.78	1.14
1:B:651:MET:HG2	1:B:670:MET:HE1	1.24	1.14
1:B:33:TYR:OH	1:B:264:ASN:ND2	1.81	1.12
1:B:178:LEU:C	1:B:211:ARG:HH12	1.60	1.08
1:A:30:ILE:O	1:A:34:THR:OG1	1.76	1.03
1:A:179:VAL:HG21	1:A:241:LYS:HD3	1.02	1.02
1:B:18:HIS:CD2	1:B:19:ILE:H	1.76	1.02
1:B:113:GLU:OE1	1:B:115:GLN:N	1.93	1.01
1:B:659:ARG:HH11	1:B:659:ARG:HG3	1.20	1.00
1:B:222:SER:HB3	1:B:225:LEU:HD21	1.42	1.00
1:A:216:GLU:O	1:A:219:ALA:N	1.94	0.99
1:A:300:ILE:HG12	1:A:302:LYS:HD2	1.41	0.99
1:A:534:PRO:HD3	1:A:571:TYR:CD2	1.98	0.98
1:A:199:ILE:HD12	1:A:199:ILE:H	1.27	0.95
1:A:304:ASP:OD1	1:A:307:ALA:N	2.00	0.94
1:A:179:VAL:CG2	1:A:241:LYS:HD3	1.97	0.92
1:B:178:LEU:O	1:B:211:ARG:NH1	2.03	0.90
1:A:622:ASP:OD1	1:A:626:ARG:NH1	2.04	0.89
1:B:109:GLN:HG3	1:B:110:SER:N	1.86	0.89
1:B:33:TYR:HH	1:B:264:ASN:ND2	1.69	0.89
1:A:417:LYS:NZ	1:A:421:ASP:OD1	2.05	0.89
1:B:230:LEU:HD23	1:B:230:LEU:H	1.38	0.89
1:A:534:PRO:HD3	1:A:571:TYR:HD2	1.32	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:651:MET:CG	1:B:670:MET:HE1	2.05	0.87
1:A:117:GLU:OE2	1:A:154:ARG:NH2	2.07	0.87
1:A:572:HIS:HD2	1:A:573:ASP:H	1.21	0.87
1:A:241:LYS:NZ	1:A:277:TYR:OH	2.06	0.87
1:A:409:HIS:HD2	1:A:481:SER:HB3	1.38	0.87
1:B:611:MET:SD	1:B:619:ILE:HG13	2.16	0.86
1:B:659:ARG:O	1:B:663:GLN:N	2.09	0.85
1:A:394:ASN:OD1	1:A:395:ASP:N	2.11	0.84
1:B:658:LEU:O	1:B:662:THR:HG22	1.77	0.84
1:B:90:VAL:HG23	1:B:91:GLU:H	1.42	0.83
1:B:342:LYS:NZ	1:B:394:ASN:O	2.11	0.83
1:B:164:LEU:HB2	1:B:176:ILE:HD11	1.61	0.83
1:B:112:VAL:HG21	1:B:155:LEU:HD11	1.61	0.83
1:A:392:GLU:OE1	1:A:392:GLU:N	2.12	0.82
1:A:287:ILE:HD13	1:A:398:LEU:HD23	1.61	0.82
1:A:413:GLU:HB3	1:A:474:ASN:HB2	1.60	0.82
1:A:300:ILE:CG1	1:A:302:LYS:HD2	2.10	0.81
1:A:179:VAL:HG21	1:A:241:LYS:CD	1.99	0.81
1:B:534:PRO:HG2	1:B:537:TYR:HD2	1.46	0.80
1:B:178:LEU:C	1:B:211:ARG:NH1	2.38	0.80
1:B:115:GLN:O	1:B:118:THR:OG1	1.99	0.80
1:A:495:LYS:HD3	1:A:508:ASP:HB2	1.64	0.80
1:A:286:PRO:HB3	1:A:302:LYS:HG3	1.64	0.79
1:B:488:SER:HB2	1:B:596:CYS:HA	1.63	0.79
1:B:633:MET:HE3	1:B:640:GLN:HG2	1.64	0.79
1:A:268:GLN:OE1	1:A:268:GLN:N	2.15	0.78
1:A:686:ILE:O	1:A:690:ASN:ND2	2.16	0.78
1:B:180:GLU:HG2	1:B:182:LYS:HE3	1.66	0.78
1:B:659:ARG:HG3	1:B:659:ARG:NH1	1.88	0.78
1:A:335:MET:HE2	1:A:352:VAL:HG21	1.64	0.78
1:B:191:GLY:HA3	1:B:264:ASN:HD22	1.47	0.77
1:A:683:ALA:HA	1:A:686:ILE:HD12	1.65	0.77
1:B:219:ALA:HA	1:B:225:LEU:HD12	1.66	0.77
1:A:508:ASP:OD2	1:A:570:SER:N	2.18	0.77
1:A:166:ILE:HD12	1:A:174:ALA:HB3	1.66	0.76
1:A:308:GLU:OE1	1:A:394:ASN:HB2	1.85	0.76
1:A:260:THR:HG22	1:A:263:LYS:H	1.50	0.76
1:B:18:HIS:HD2	1:B:19:ILE:H	1.27	0.76
1:B:688:LYS:O	1:B:691:LYS:HG2	1.84	0.76
1:B:83:PRO:HG2	1:B:92:VAL:HG23	1.67	0.76
1:A:493:GLN:OE1	1:A:510:HIS:NE2	2.19	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:547:ASP:O	1:A:551:ASN:ND2	2.19	0.75
1:B:154:ARG:HD3	1:B:636:ARG:NH2	2.02	0.74
1:B:464:ARG:O	1:B:468:GLU:HB3	1.87	0.74
1:B:163:GLN:CD	1:B:175:ILE:HD11	2.11	0.74
1:B:626:ARG:NH1	1:B:650:GLU:O	2.20	0.74
1:A:414:PRO:HG3	1:A:423:MET:HE1	1.68	0.74
1:B:510:HIS:HB2	1:B:568:ASP:HB3	1.69	0.74
1:B:164:LEU:H	1:B:176:ILE:CD1	1.99	0.74
1:B:523:GLU:HB2	1:B:563:LYS:HE2	1.69	0.74
1:A:241:LYS:O	1:A:244:ILE:HG13	1.86	0.74
1:A:619:ILE:O	1:A:622:ASP:HB3	1.86	0.74
1:A:209:GLU:O	1:A:213:SER:OG	2.06	0.73
1:B:224:GLU:HG3	1:B:225:LEU:H	1.54	0.73
1:B:651:MET:HG2	1:B:670:MET:CE	2.13	0.73
1:B:109:GLN:HG3	1:B:110:SER:H	1.52	0.72
1:B:124:THR:HG23	1:B:130:ARG:HH12	1.53	0.72
1:A:612:PRO:HG2	1:A:615:TYR:CD2	2.24	0.72
1:B:180:GLU:CG	1:B:182:LYS:HE3	2.20	0.72
1:A:538:ILE:CG2	1:A:539:PRO:HD3	2.20	0.71
1:B:17:ALA:HB3	1:B:23:LYS:HD2	1.72	0.71
1:B:18:HIS:CD2	1:B:19:ILE:N	2.55	0.71
1:B:144:PHE:CD2	1:B:165:PRO:HD3	2.25	0.71
1:A:572:HIS:CD2	1:A:573:ASP:H	2.06	0.71
1:B:226:MET:O	1:B:230:LEU:HD21	1.91	0.71
1:A:239:GLU:HA	1:A:242:GLU:OE1	1.90	0.71
1:A:505:GLN:O	1:A:505:GLN:HG2	1.91	0.71
1:B:404:PRO:HB3	1:B:453:MET:HE2	1.73	0.71
1:A:612:PRO:HG2	1:A:615:TYR:HD2	1.56	0.71
1:A:274:VAL:HG13	1:A:278:LEU:HD12	1.72	0.70
1:A:572:HIS:NE2	1:A:574:VAL:HG12	2.06	0.70
1:A:361:ASN:O	1:A:362:SER:HB3	1.91	0.70
1:B:419:ASP:HA	1:B:422:LYS:HE2	1.73	0.70
1:A:535:ARG:O	1:A:538:ILE:HG22	1.92	0.70
1:A:529:VAL:HG13	1:A:530:GLY:H	1.56	0.70
1:A:201:GLU:CD	1:A:201:GLU:H	1.96	0.70
1:A:411:SER:HA	1:A:449:ILE:HD13	1.75	0.69
1:B:278:LEU:HB3	1:B:279:PRO:HD2	1.73	0.69
1:B:224:GLU:HG3	1:B:225:LEU:HD23	1.73	0.69
1:B:373:ASP:OD1	1:B:374:ILE:N	2.25	0.69
1:B:414:PRO:HG3	1:B:420:GLN:HG3	1.74	0.69
1:A:311:ALA:HB2	1:A:330:VAL:HG12	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:302:LYS:HE3	1:B:304:ASP:HB2	1.75	0.69
1:B:620:MET:HE1	1:B:630:VAL:HG21	1.74	0.69
1:A:409:HIS:CD2	1:A:481:SER:HB3	2.26	0.69
1:A:276:ASP:HB3	1:A:277:TYR:CE1	2.29	0.68
1:A:304:ASP:OD1	1:A:306:SER:N	2.26	0.68
1:A:350:GLU:HG2	1:A:380:LEU:HG	1.74	0.68
1:B:8:GLU:OE1	1:B:8:GLU:N	2.21	0.68
1:A:578:GLU:OE2	1:A:579:MET:HG2	1.94	0.67
1:A:633:MET:SD	1:A:640:GLN:HG2	2.34	0.67
1:B:223:ASP:O	1:B:226:MET:HG2	1.94	0.67
1:A:3:ARG:HB3	1:A:370:TYR:CD2	2.29	0.67
1:B:260:THR:CG2	1:B:263:LYS:HB2	2.25	0.67
1:A:354:ARG:HD2	1:A:365:GLU:OE1	1.93	0.67
1:B:227:GLU:O	1:B:230:LEU:HG	1.93	0.67
1:B:433:GLU:OE1	1:B:464:ARG:NH2	2.25	0.67
1:B:176:ILE:H	1:B:176:ILE:HD12	1.59	0.67
1:A:218:VAL:O	1:A:221:THR:OG1	2.11	0.67
1:B:688:LYS:HA	1:B:691:LYS:HG2	1.77	0.67
1:A:612:PRO:HB2	1:A:614:GLU:CD	2.20	0.66
1:B:319:ASP:OD1	1:B:320:PRO:HD2	1.95	0.66
1:B:162:ILE:HG13	1:B:163:GLN:HG3	1.77	0.66
1:A:622:ASP:O	1:A:625:SER:OG	2.09	0.65
1:A:622:ASP:CG	1:A:626:ARG:HH12	2.04	0.65
1:A:505:GLN:N	1:A:575:ASP:HB3	2.12	0.65
1:B:133:PHE:HD2	1:B:270:MET:HG3	1.61	0.65
1:A:297:GLU:H	1:A:297:GLU:CD	2.03	0.65
1:A:181:MET:HG2	1:A:211:ARG:HH11	1.61	0.65
1:A:97:ARG:NH2	1:A:287:ILE:HD11	2.12	0.65
1:B:535:ARG:HG2	1:B:535:ARG:HH11	1.61	0.65
1:A:414:PRO:HG3	1:A:423:MET:CE	2.27	0.65
1:A:516:ASN:OD1	1:A:517:GLU:N	2.27	0.65
1:B:441:THR:O	1:B:442:ASP:HB3	1.95	0.65
1:A:117:GLU:HB3	1:A:155:LEU:HD11	1.79	0.65
1:A:309:PHE:HA	1:A:333:GLY:HA3	1.78	0.65
1:A:505:GLN:N	1:A:505:GLN:HE21	1.95	0.64
1:B:346:LYS:HG3	1:B:348:LYS:NZ	2.12	0.64
1:B:447:GLN:OE1	1:B:447:GLN:N	2.30	0.64
1:A:604:MET:HE1	1:A:647:PRO:HG3	1.79	0.64
1:B:228:LYS:HE2	1:B:233:GLU:O	1.97	0.64
1:B:553:VAL:HG23	1:B:554:LEU:H	1.63	0.64
1:A:201:GLU:CD	1:A:201:GLU:N	2.55	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:ASN:ND2	1:A:192:THR:O	2.30	0.64
1:B:257:LEU:HD22	1:B:270:MET:HA	1.80	0.64
1:B:316:VAL:HG23	1:B:433:GLU:HG2	1.79	0.64
1:A:15:ILE:HD11	1:A:30:ILE:HD12	1.79	0.64
1:A:156:GLN:NE2	1:A:637:GLY:HA3	2.12	0.64
1:B:211:ARG:O	1:B:214:LEU:HB3	1.98	0.64
1:B:341:VAL:HG12	1:B:342:LYS:N	2.13	0.63
1:B:83:PRO:HG3	1:B:91:GLU:HB3	1.79	0.63
1:B:151:LEU:HA	1:B:155:LEU:HD13	1.80	0.63
1:B:346:LYS:HE2	1:B:348:LYS:HZ1	1.62	0.63
1:B:436:THR:HB	1:B:453:MET:HE3	1.80	0.63
1:A:572:HIS:CD2	1:A:573:ASP:N	2.66	0.63
1:B:659:ARG:HH11	1:B:659:ARG:CG	2.01	0.63
1:A:284:VAL:HG22	1:A:285:LYS:N	2.14	0.63
1:A:572:HIS:HD2	1:A:573:ASP:N	1.92	0.62
1:B:346:LYS:HG3	1:B:348:LYS:HZ3	1.63	0.62
1:A:549:MET:HE3	1:A:559:LEU:HD23	1.82	0.62
1:B:234:GLU:HA	1:B:234:GLU:OE1	1.98	0.62
1:B:90:VAL:HG23	1:B:91:GLU:N	2.13	0.62
1:B:237:VAL:O	1:B:240:LEU:N	2.31	0.62
1:A:228:LYS:HA	1:A:233:GLU:HG3	1.82	0.62
1:A:244:ILE:CD1	1:A:277:TYR:CE1	2.83	0.62
1:B:179:VAL:HA	1:B:211:ARG:HH22	1.64	0.62
1:A:361:ASN:OD1	1:A:361:ASN:N	2.30	0.61
1:A:73:GLU:O	1:A:75:HIS:ND1	2.29	0.61
1:A:622:ASP:CG	1:A:626:ARG:NH1	2.57	0.61
1:A:291:ARG:HG3	1:A:297:GLU:HG3	1.82	0.61
1:A:297:GLU:OE1	1:A:297:GLU:N	2.19	0.61
1:A:146:TYR:CD1	1:A:146:TYR:C	2.76	0.61
1:A:164:LEU:HD11	1:A:178:LEU:HD11	1.82	0.61
1:B:88:LEU:HD13	1:B:91:GLU:OE1	2.01	0.61
1:A:318:THR:OG1	1:A:429:LYS:NZ	2.30	0.60
1:A:115:GLN:H	1:A:115:GLN:CD	2.08	0.60
1:A:234:GLU:OE1	1:A:234:GLU:HA	1.98	0.60
1:B:341:VAL:HG12	1:B:342:LYS:H	1.66	0.60
1:A:346:LYS:NZ	1:A:387:ASP:OD2	2.34	0.60
1:B:335:MET:HG2	1:B:336:THR:N	2.15	0.60
1:B:646:VAL:HG11	1:B:651:MET:HE1	1.82	0.60
1:B:201:GLU:HG2	1:B:202:ASP:N	2.15	0.60
1:B:276:ASP:HB3	1:B:277:TYR:CD1	2.37	0.60
1:B:620:MET:CE	1:B:630:VAL:HG21	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:THR:O	1:A:30:ILE:HG13	2.01	0.60
1:A:216:GLU:HA	1:A:219:ALA:HB3	1.83	0.60
1:B:291:ARG:HB3	1:B:395:ASP:OD2	2.02	0.60
1:B:607:VAL:HG22	1:B:670:MET:HE2	1.83	0.60
1:B:276:ASP:HB3	1:B:277:TYR:CE1	2.36	0.60
1:A:201:GLU:N	1:A:201:GLU:OE1	2.35	0.60
1:B:144:PHE:HD2	1:B:165:PRO:CD	2.15	0.60
1:B:614:GLU:HG2	1:B:615:TYR:CD1	2.36	0.60
1:A:487:LYS:HD2	1:A:599:VAL:HG11	1.83	0.60
1:A:284:VAL:HG22	1:A:285:LYS:H	1.67	0.59
1:A:538:ILE:HG23	1:A:539:PRO:HD3	1.84	0.59
1:A:491:GLN:HG2	1:A:512:GLU:HG3	1.85	0.59
1:B:211:ARG:O	1:B:215:ILE:HG13	2.02	0.59
1:A:188:ASN:HD21	1:A:192:THR:C	2.08	0.59
1:B:85:HIS:O	1:B:88:LEU:HD12	2.02	0.59
1:B:171:GLU:O	1:B:173:GLU:HG3	2.02	0.59
1:A:3:ARG:HB3	1:A:370:TYR:CE2	2.37	0.59
1:B:224:GLU:HG3	1:B:225:LEU:N	2.18	0.59
1:B:237:VAL:HG23	1:B:238:SER:H	1.67	0.59
1:B:633:MET:CE	1:B:640:GLN:HG2	2.32	0.59
1:A:574:VAL:HG13	1:A:575:ASP:N	2.16	0.59
1:A:28:GLU:HG3	1:A:29:ARG:N	2.17	0.59
1:A:508:ASP:OD1	1:A:509:VAL:N	2.36	0.58
1:A:506:TYR:OH	1:A:570:SER:OG	2.10	0.58
1:B:553:VAL:HG23	1:B:554:LEU:N	2.18	0.58
1:A:179:VAL:HG11	1:A:241:LYS:HZ3	1.67	0.58
1:B:164:LEU:H	1:B:176:ILE:HD12	1.68	0.58
1:B:222:SER:HB3	1:B:225:LEU:CD2	2.24	0.58
1:A:106:LEU:HD11	1:A:151:LEU:HD11	1.84	0.58
1:B:7:LEU:HD22	1:B:281:PRO:HG2	1.86	0.58
1:B:534:PRO:HG2	1:B:537:TYR:CD2	2.33	0.57
1:A:147:SER:O	1:A:150:THR:OG1	2.22	0.57
1:A:88:LEU:O	1:A:92:VAL:HG23	2.05	0.57
1:A:107:ASP:OD2	1:A:139:LYS:NZ	2.38	0.57
1:A:244:ILE:O	1:A:247:ALA:N	2.38	0.57
1:B:616:MET:HE1	1:B:620:MET:HG3	1.85	0.57
1:A:17:ALA:HB2	1:A:105:VAL:HB	1.87	0.57
1:A:631:ASP:HA	1:B:635:PRO:HD3	1.87	0.57
1:A:144:PHE:O	1:A:148:VAL:HG23	2.05	0.57
1:B:120:TRP:CG	1:B:155:LEU:HD23	2.39	0.57
1:B:419:ASP:OD1	1:B:472:GLU:OE1	2.21	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:LEU:CB	1:B:176:ILE:HD11	2.33	0.56
1:A:300:ILE:HG12	1:A:302:LYS:CD	2.28	0.56
1:A:251:VAL:HG22	1:A:251:VAL:O	2.04	0.56
1:B:94:ARG:HG3	1:B:399:GLU:OE2	2.05	0.56
1:B:132:VAL:HB	1:B:256:VAL:HG22	1.86	0.56
1:B:343:ASN:N	1:B:348:LYS:O	2.34	0.56
1:B:447:GLN:O	1:B:447:GLN:HG2	2.05	0.56
1:B:525:GLU:CD	1:B:565:LYS:HE2	2.31	0.56
1:B:549:MET:HE3	1:B:559:LEU:HD23	1.87	0.56
1:B:574:VAL:HG22	1:B:575:ASP:N	2.20	0.56
1:A:538:ILE:HG22	1:A:539:PRO:HD3	1.87	0.56
1:A:682:ILE:HG22	1:A:686:ILE:HD11	1.88	0.56
1:A:266:GLY:H	1:A:268:GLN:HE22	1.53	0.56
1:B:176:ILE:HG22	1:B:182:LYS:O	2.05	0.56
1:B:337:SER:HA	1:B:352:VAL:HG12	1.88	0.56
1:B:487:LYS:HE2	1:B:599:VAL:CG1	2.35	0.56
1:B:555:ALA:CB	1:B:557:TYR:HD2	2.19	0.56
1:A:686:ILE:HG22	1:A:690:ASN:HD21	1.71	0.56
1:A:199:ILE:H	1:A:199:ILE:CD1	2.03	0.56
1:B:342:LYS:HD3	1:B:392:GLU:HA	1.88	0.56
1:A:204:LEU:O	1:A:208:GLU:HG2	2.06	0.56
1:A:304:ASP:OD1	1:A:304:ASP:C	2.48	0.55
1:A:408:ILE:HD11	1:A:478:PRO:HB3	1.87	0.55
1:A:620:MET:C	1:A:622:ASP:N	2.63	0.55
1:B:222:SER:CB	1:B:225:LEU:HD21	2.25	0.55
1:A:11:ARG:NH2	1:A:275:ILE:O	2.28	0.55
1:B:319:ASP:HB3	1:B:322:VAL:HG22	1.88	0.55
1:B:441:THR:HG23	1:B:442:ASP:N	2.21	0.55
1:A:294:ASN:O	1:A:297:GLU:CD	2.50	0.55
1:B:143:ASN:ND2	1:B:146:TYR:HB2	2.21	0.55
1:B:177:ASP:O	1:B:181:MET:N	2.40	0.55
1:B:342:LYS:HA	1:B:349:ARG:HA	1.87	0.55
1:B:512:GLU:OE2	1:B:565:LYS:HD2	2.07	0.55
1:A:260:THR:HG21	1:A:263:LYS:HG2	1.88	0.55
1:B:144:PHE:CD2	1:B:165:PRO:CD	2.88	0.55
1:B:250:ASN:HB2	1:B:252:GLU:HG2	1.89	0.55
1:B:431:GLN:NE2	1:B:435:PRO:HA	2.22	0.55
1:A:611:MET:HE1	1:A:642:VAL:HG23	1.88	0.55
1:B:538:ILE:N	1:B:539:PRO:HD2	2.22	0.55
1:A:143:ASN:HB3	1:A:146:TYR:HB3	1.88	0.54
1:A:620:MET:O	1:A:623:VAL:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:LEU:O	1:B:181:MET:N	2.40	0.54
1:B:687:ILE:C	1:B:691:LYS:HZ2	2.15	0.54
1:A:117:GLU:O	1:A:121:ARG:HG3	2.08	0.54
1:B:260:THR:HG23	1:B:263:LYS:HB2	1.89	0.54
1:B:688:LYS:CG	1:B:689:LYS:N	2.71	0.54
1:A:529:VAL:HG13	1:A:530:GLY:N	2.20	0.54
1:B:164:LEU:N	1:B:176:ILE:CD1	2.70	0.54
1:A:164:LEU:CD1	1:A:178:LEU:HD21	2.37	0.54
1:A:227:GLU:HA	1:A:230:LEU:HD11	1.89	0.54
1:B:237:VAL:O	1:B:240:LEU:HB3	2.08	0.54
1:A:120:TRP:CD2	1:A:155:LEU:HD23	2.43	0.54
1:B:89:THR:O	1:B:93:GLU:HB2	2.07	0.54
1:A:276:ASP:CB	1:A:277:TYR:CE1	2.90	0.54
1:B:349:ARG:NH1	1:B:392:GLU:OE1	2.41	0.54
1:B:535:ARG:HH11	1:B:535:ARG:CG	2.21	0.54
1:A:227:GLU:C	1:A:227:GLU:OE1	2.51	0.54
1:A:335:MET:HE3	1:A:336:THR:O	2.08	0.54
1:B:247:ALA:HA	1:B:252:GLU:HG3	1.90	0.53
1:B:651:MET:HE2	1:B:651:MET:CA	2.38	0.53
1:A:289:GLY:O	1:A:299:VAL:N	2.28	0.53
1:B:3:ARG:HD2	1:B:370:TYR:CD2	2.43	0.53
1:A:268:GLN:H	1:A:268:GLN:CD	2.10	0.53
1:B:547:ASP:O	1:B:550:GLU:N	2.41	0.53
1:A:636:ARG:HG2	1:A:636:ARG:O	2.08	0.53
1:A:186:TYR:CE2	1:A:265:LYS:HA	2.43	0.53
1:B:615:TYR:CD2	1:B:662:THR:HA	2.44	0.53
1:A:212:ALA:O	1:A:215:ILE:HG12	2.09	0.53
1:A:362:SER:O	1:A:363:ARG:HG3	2.09	0.53
1:A:635:PRO:HB3	1:A:640:GLN:NE2	2.24	0.53
1:B:31:LEU:HD23	1:B:79:ILE:HD12	1.91	0.53
1:B:138:ASP:HA	1:B:169:GLU:O	2.08	0.53
1:A:537:TYR:OH	1:A:577:SER:HA	2.09	0.53
1:B:120:TRP:CD1	1:B:155:LEU:HD23	2.43	0.53
1:B:629:ARG:HG3	1:B:630:VAL:N	2.24	0.52
1:A:330:VAL:HG21	1:A:370:TYR:O	2.08	0.52
1:B:147:SER:O	1:B:150:THR:OG1	2.21	0.52
1:A:322:VAL:HG13	1:A:354:ARG:NH2	2.25	0.52
1:A:616:MET:SD	1:A:633:MET:HE1	2.50	0.52
1:B:516:ASN:OD1	1:B:517:GLU:N	2.42	0.52
1:B:545:LEU:O	1:B:549:MET:HG3	2.10	0.52
1:A:419:ASP:HB3	1:A:471:VAL:HG13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:HIS:HA	1:A:297:GLU:O	2.09	0.52
1:A:505:GLN:N	1:A:505:GLN:NE2	2.57	0.52
1:B:101:GLY:HA2	1:B:128:VAL:HG13	1.91	0.52
1:B:222:SER:HB3	1:B:225:LEU:HD11	1.91	0.52
1:A:216:GLU:OE1	1:A:216:GLU:N	2.33	0.52
1:A:505:GLN:O	1:A:505:GLN:CG	2.57	0.52
1:A:468:GLU:CD	1:A:469:PHE:HE1	2.18	0.52
1:B:103:VAL:HG22	1:B:131:ILE:HG12	1.92	0.52
1:B:535:ARG:HB2	1:B:535:ARG:CZ	2.39	0.52
1:A:231:GLY:O	1:A:232:ASP:HB3	2.10	0.52
1:B:223:ASP:HA	1:B:226:MET:HE2	1.92	0.52
1:A:325:LEU:HD22	1:A:376:ALA:HB1	1.91	0.51
1:B:225:LEU:O	1:B:228:LYS:N	2.43	0.51
1:B:488:SER:HB2	1:B:596:CYS:CA	2.38	0.51
1:A:85:HIS:HE1	1:A:87:ASP:CG	2.18	0.51
1:A:622:ASP:OD2	1:A:654:TYR:HE1	1.92	0.51
1:B:31:LEU:HD22	1:B:68:THR:HG21	1.92	0.51
1:B:618:ASP:OD1	1:B:618:ASP:N	2.38	0.51
1:A:284:VAL:CG2	1:A:285:LYS:H	2.23	0.51
1:A:404:PRO:O	1:A:405:GLU:HB2	2.10	0.51
1:B:572:HIS:CE1	1:B:574:VAL:HG13	2.45	0.51
1:A:106:LEU:HD22	1:A:112:VAL:HA	1.93	0.51
1:A:236:SER:HB3	1:A:239:GLU:HG2	1.91	0.51
1:A:609:ILE:HG22	1:A:610:GLU:N	2.26	0.51
1:B:440:HIS:O	1:B:448:VAL:HG23	2.10	0.51
1:B:163:GLN:O	1:B:164:LEU:HD12	2.10	0.51
1:A:18:HIS:CG	1:A:19:ILE:H	2.28	0.51
1:A:352:VAL:CG1	1:A:355:LEU:HD21	2.41	0.51
1:A:434:ASP:OD1	1:A:436:THR:OG1	2.16	0.51
1:B:651:MET:HE2	1:B:651:MET:HA	1.91	0.51
1:A:117:GLU:OE2	1:A:154:ARG:CZ	2.58	0.51
1:A:216:GLU:O	1:A:217:ALA:C	2.54	0.51
1:B:86:VAL:HG12	1:B:86:VAL:O	2.11	0.51
1:A:294:ASN:O	1:A:297:GLU:OE1	2.29	0.51
1:A:496:PHE:O	1:A:506:TYR:HA	2.11	0.51
1:A:85:HIS:CE1	1:A:87:ASP:CG	2.89	0.50
1:B:616:MET:HE1	1:B:620:MET:CG	2.40	0.50
1:A:463:ASP:O	1:A:467:LYS:HD2	2.11	0.50
1:A:31:LEU:HD23	1:A:79:ILE:HD12	1.92	0.50
1:A:146:TYR:C	1:A:146:TYR:HD1	2.19	0.50
1:A:244:ILE:HD13	1:A:277:TYR:CE1	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:GLN:NE2	1:A:246:GLN:HA	2.26	0.50
1:B:101:GLY:HA2	1:B:128:VAL:CG1	2.42	0.50
1:B:688:LYS:HA	1:B:691:LYS:CG	2.40	0.50
1:A:18:HIS:O	1:A:23:LYS:HB2	2.12	0.50
1:A:181:MET:HG2	1:A:211:ARG:NH1	2.24	0.50
1:A:626:ARG:HG3	1:A:626:ARG:HH11	1.76	0.50
1:B:555:ALA:HB3	1:B:557:TYR:HD2	1.76	0.50
1:A:605:MET:HB3	1:A:670:MET:HG3	1.93	0.50
1:A:270:MET:O	1:A:273:ALA:HB3	2.12	0.50
1:A:352:VAL:HG12	1:A:353:GLY:O	2.12	0.50
1:B:308:GLU:OE2	1:B:394:ASN:ND2	2.45	0.50
1:B:554:LEU:HD23	1:B:600:ILE:HG13	1.92	0.50
1:A:120:TRP:CG	1:A:155:LEU:HD23	2.47	0.50
1:A:276:ASP:C	1:A:277:TYR:CD1	2.90	0.50
1:B:112:VAL:HG11	1:B:155:LEU:CD1	2.42	0.49
1:B:138:ASP:O	1:B:139:LYS:HB2	2.12	0.49
1:B:225:LEU:O	1:B:226:MET:C	2.53	0.49
1:B:396:ILE:C	1:B:397:ILE:HG12	2.37	0.49
1:B:404:PRO:CB	1:B:453:MET:HE2	2.40	0.49
1:A:18:HIS:CG	1:A:19:ILE:N	2.80	0.49
1:A:460:ILE:HA	1:A:463:ASP:HB3	1.95	0.49
1:A:224:GLU:O	1:A:228:LYS:HG3	2.13	0.49
1:B:343:ASN:HA	1:B:389:LEU:HD23	1.95	0.49
1:A:114:PRO:O	1:A:118:THR:HG23	2.13	0.49
1:A:230:LEU:C	1:A:232:ASP:N	2.70	0.49
1:B:550:GLU:N	1:B:550:GLU:OE1	2.46	0.49
1:A:671:TYR:N	1:A:671:TYR:CD1	2.81	0.49
1:B:662:THR:C	1:B:663:GLN:OE1	2.56	0.49
1:B:662:THR:O	1:B:663:GLN:HB2	2.12	0.49
1:B:191:GLY:CA	1:B:264:ASN:HD22	2.23	0.49
1:A:226:MET:O	1:A:230:LEU:HG	2.12	0.48
1:A:284:VAL:CG2	1:A:285:LYS:N	2.76	0.48
1:A:294:ASN:O	1:A:297:GLU:OE2	2.31	0.48
1:B:523:GLU:CB	1:B:563:LYS:HE2	2.42	0.48
1:A:426:ALA:HB2	1:A:469:PHE:CD2	2.47	0.48
1:A:463:ASP:OD2	1:A:467:LYS:NZ	2.32	0.48
1:A:532:VAL:HG12	1:A:570:SER:HA	1.96	0.48
1:A:574:VAL:CG1	1:A:575:ASP:N	2.76	0.48
1:B:178:LEU:O	1:B:179:VAL:C	2.56	0.48
1:B:413:GLU:HB3	1:B:474:ASN:OD1	2.13	0.48
1:B:441:THR:HG23	1:B:442:ASP:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:677:GLU:HG2	1:B:678:VAL:H	1.79	0.48
1:A:532:VAL:HG11	1:A:569:GLY:O	2.13	0.48
1:A:286:PRO:CG	1:A:300:ILE:HD11	2.44	0.48
1:B:164:LEU:HD11	1:B:210:ALA:HB1	1.94	0.48
1:B:621:GLY:O	1:B:625:SER:OG	2.31	0.48
1:B:119:VAL:O	1:B:123:ALA:N	2.44	0.48
1:B:683:ALA:O	1:B:687:ILE:HG13	2.14	0.48
1:A:309:PHE:CD1	1:A:309:PHE:C	2.91	0.48
1:A:407:VAL:HG11	1:A:672:PHE:CD1	2.49	0.48
1:B:505:GLN:O	1:B:505:GLN:HG2	2.13	0.48
1:B:688:LYS:CA	1:B:691:LYS:HG2	2.43	0.48
1:A:308:GLU:CD	1:A:394:ASN:HB2	2.39	0.48
1:A:532:VAL:CG1	1:A:569:GLY:O	2.62	0.48
1:A:571:TYR:CD1	1:A:571:TYR:C	2.92	0.48
1:B:181:MET:HE3	1:B:199:ILE:HD12	1.95	0.48
1:B:452:GLY:HA3	1:B:458:LEU:HD21	1.96	0.48
1:B:174:ALA:HB1	1:B:184:PHE:O	2.14	0.48
1:A:194:ILE:HG13	1:A:194:ILE:O	2.14	0.47
1:A:457:HIS:O	1:A:460:ILE:HG13	2.13	0.47
1:B:413:GLU:O	1:B:474:ASN:OD1	2.32	0.47
1:A:205:ASP:O	1:A:209:GLU:OE1	2.32	0.47
1:A:433:GLU:OE1	1:A:464:ARG:NH1	2.46	0.47
1:A:618:ASP:OD1	1:A:618:ASP:N	2.47	0.47
1:B:168:ALA:O	1:B:171:GLU:N	2.46	0.47
1:B:186:TYR:CD2	1:B:265:LYS:HG2	2.49	0.47
1:B:337:SER:HA	1:B:352:VAL:CG1	2.44	0.47
1:A:572:HIS:CE1	1:A:574:VAL:HG12	2.49	0.47
1:B:121:ARG:HA	1:B:124:THR:OG1	2.14	0.47
1:B:146:TYR:O	1:B:150:THR:HG23	2.14	0.47
1:B:214:LEU:O	1:B:218:VAL:HG23	2.15	0.47
1:A:3:ARG:HH22	1:A:7:LEU:HD23	1.79	0.47
1:A:324:LYS:CE	1:A:380:LEU:O	2.61	0.47
1:A:509:VAL:HG22	1:A:584:ALA:HB1	1.96	0.47
1:B:7:LEU:HD22	1:B:281:PRO:CG	2.44	0.47
1:A:101:GLY:HA2	1:A:128:VAL:HG13	1.96	0.47
1:A:146:TYR:O	1:A:149:SER:N	2.45	0.47
1:A:163:GLN:HA	1:A:176:ILE:O	2.15	0.47
1:A:251:VAL:HG23	1:A:254:TYR:CE1	2.50	0.47
1:B:240:LEU:O	1:B:244:ILE:HG13	2.15	0.47
1:B:241:LYS:HA	1:B:244:ILE:HD12	1.97	0.47
1:A:34:THR:HG22	1:A:71:ALA:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:549:MET:HB3	1:A:559:LEU:HB3	1.96	0.47
1:B:83:PRO:HG3	1:B:91:GLU:CB	2.44	0.47
1:B:309:PHE:O	1:B:390:CYS:HA	2.14	0.47
1:B:354:ARG:HE	1:B:365:GLU:CD	2.23	0.47
1:B:450:ILE:HG13	1:B:450:ILE:O	2.14	0.47
1:B:237:VAL:HG23	1:B:238:SER:N	2.30	0.46
1:A:426:ALA:HB2	1:A:469:PHE:HD2	1.80	0.46
1:A:538:ILE:HG23	1:A:539:PRO:CD	2.45	0.46
1:B:484:GLU:OE2	1:B:555:ALA:HB3	2.15	0.46
1:B:677:GLU:HG2	1:B:678:VAL:N	2.30	0.46
1:A:25:THR:O	1:A:29:ARG:HG2	2.14	0.46
1:A:441:THR:O	1:A:442:ASP:C	2.58	0.46
1:A:554:LEU:HD22	1:A:598:PRO:HB2	1.98	0.46
1:B:287:ILE:HG22	1:B:301:ALA:HB3	1.98	0.46
1:A:146:TYR:O	1:A:149:SER:OG	2.26	0.46
1:B:405:GLU:HG3	1:B:406:PRO:HD2	1.96	0.46
1:A:120:TRP:CD1	1:A:120:TRP:C	2.93	0.46
1:A:487:LYS:CD	1:A:599:VAL:HG11	2.46	0.46
1:B:34:THR:HB	1:B:70:ALA:HB1	1.98	0.46
1:B:112:VAL:HG11	1:B:155:LEU:HD11	1.97	0.46
1:A:149:SER:O	1:A:152:HIS:HB2	2.15	0.46
1:A:201:GLU:O	1:A:204:LEU:HB2	2.16	0.46
1:B:202:ASP:N	1:B:202:ASP:OD1	2.41	0.46
1:A:330:VAL:HG21	1:A:369:VAL:CG1	2.46	0.46
1:A:396:ILE:HG12	1:A:397:ILE:N	2.31	0.46
1:B:154:ARG:HB3	1:B:155:LEU:HD12	1.96	0.46
1:B:397:ILE:HG22	1:B:398:LEU:N	2.31	0.46
1:A:524:PHE:CD1	1:A:524:PHE:C	2.93	0.46
1:B:278:LEU:HB3	1:B:279:PRO:CD	2.42	0.46
1:B:626:ARG:O	1:B:627:ARG:HB2	2.15	0.46
1:A:113:GLU:HB3	1:A:114:PRO:HD2	1.98	0.46
1:B:477:ALA:HA	1:B:478:PRO:HD3	1.75	0.45
1:A:32:TYR:CD1	1:A:32:TYR:C	2.94	0.45
1:A:205:ASP:O	1:A:208:GLU:N	2.49	0.45
1:B:540:SER:O	1:B:582:LYS:HG3	2.15	0.45
1:A:230:LEU:HG	1:A:230:LEU:H	1.52	0.45
1:A:268:GLN:N	1:A:268:GLN:CD	2.73	0.45
1:A:291:ARG:HG2	1:A:299:VAL:HG21	1.97	0.45
1:B:179:VAL:CA	1:B:211:ARG:HH22	2.28	0.45
1:B:343:ASN:HA	1:B:389:LEU:CD2	2.46	0.45
1:A:216:GLU:C	1:A:219:ALA:H	2.18	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:517:GLU:HB3	1:A:520:ALA:HB2	1.99	0.45
1:B:3:ARG:HH12	1:B:7:LEU:N	2.15	0.45
1:B:154:ARG:HD3	1:B:636:ARG:CZ	2.46	0.45
1:B:230:LEU:H	1:B:230:LEU:CD2	2.08	0.45
1:B:235:ILE:HD13	1:B:235:ILE:N	2.31	0.45
1:B:496:PHE:CD1	1:B:497:SER:N	2.84	0.45
1:B:633:MET:O	1:B:634:GLU:HB3	2.15	0.45
1:A:15:ILE:CD1	1:A:30:ILE:HD12	2.46	0.45
1:A:140:LEU:C	1:A:142:ALA:N	2.74	0.45
1:B:17:ALA:HB1	1:B:23:LYS:HB2	1.99	0.45
1:B:18:HIS:CD2	1:B:19:ILE:HG22	2.52	0.45
1:B:318:THR:O	1:B:318:THR:HG22	2.17	0.45
1:A:296:GLU:N	1:A:297:GLU:OE1	2.49	0.45
1:B:112:VAL:HG12	1:B:150:THR:OG1	2.17	0.45
1:A:201:GLU:HA	1:A:204:LEU:HD12	1.99	0.45
1:A:201:GLU:HA	1:A:204:LEU:HG	1.98	0.45
1:A:244:ILE:HG13	1:A:245:ARG:H	1.80	0.45
1:B:175:ILE:HG12	1:B:176:ILE:N	2.32	0.45
1:B:187:THR:HG23	1:B:193:GLU:O	2.16	0.45
1:B:688:LYS:C	1:B:690:ASN:N	2.70	0.45
1:B:688:LYS:C	1:B:691:LYS:HG2	2.39	0.45
1:B:308:GLU:O	1:B:333:GLY:HA3	2.17	0.44
1:B:593:ALA:O	1:B:598:PRO:HD3	2.17	0.44
1:A:93:GLU:O	1:A:97:ARG:HG3	2.17	0.44
1:A:277:TYR:CD1	1:A:277:TYR:N	2.82	0.44
1:A:506:TYR:HD1	1:A:576:SER:OG	1.99	0.44
1:B:682:ILE:O	1:B:686:ILE:HG13	2.16	0.44
1:A:160:ALA:N	1:A:253:PHE:HE1	2.16	0.44
1:A:392:GLU:H	1:A:392:GLU:CD	2.13	0.44
1:B:182:LYS:HD3	1:B:196:GLU:OE2	2.17	0.44
1:A:34:THR:HB	1:A:70:ALA:HB1	2.00	0.44
1:A:388:THR:CG2	1:A:398:LEU:HD13	2.46	0.44
1:A:417:LYS:HD2	1:A:417:LYS:HA	1.77	0.44
1:A:508:ASP:O	1:A:509:VAL:HG13	2.18	0.44
1:B:289:GLY:C	1:B:299:VAL:HG12	2.42	0.44
1:B:410:LEU:O	1:B:410:LEU:HD12	2.18	0.44
1:B:526:ASN:OD1	1:B:538:ILE:HD13	2.18	0.44
1:B:659:ARG:O	1:B:662:THR:N	2.44	0.44
1:A:118:THR:O	1:A:122:GLN:HG3	2.16	0.44
1:A:179:VAL:HG11	1:A:241:LYS:NZ	2.32	0.44
1:A:201:GLU:OE1	1:A:202:ASP:OD1	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:ASP:CB	1:A:277:TYR:CD1	3.01	0.44
1:A:359:HIS:HB2	1:A:362:SER:OG	2.16	0.44
1:A:392:GLU:N	1:A:392:GLU:CD	2.75	0.44
1:A:469:PHE:CD1	1:A:469:PHE:N	2.85	0.44
1:A:633:MET:HE3	1:B:633:MET:SD	2.58	0.44
1:A:324:LYS:NZ	1:A:380:LEU:O	2.50	0.44
1:A:531:GLY:C	1:A:533:VAL:N	2.73	0.44
1:B:175:ILE:HD13	1:B:269:LEU:HD12	1.99	0.44
1:B:223:ASP:HA	1:B:226:MET:CE	2.48	0.44
1:A:572:HIS:CD2	1:A:574:VAL:H	2.35	0.44
1:B:17:ALA:HB3	1:B:23:LYS:CD	2.43	0.44
1:B:93:GLU:HG2	1:B:126:TYR:OH	2.18	0.44
1:B:456:LEU:O	1:B:459:ASP:N	2.51	0.44
1:A:236:SER:CB	1:A:239:GLU:HG2	2.48	0.43
1:A:611:MET:HE1	1:A:642:VAL:CG2	2.48	0.43
1:A:72:TRP:O	1:A:75:HIS:HB2	2.18	0.43
1:B:229:TYR:CD1	1:B:229:TYR:C	2.96	0.43
1:B:341:VAL:CG1	1:B:342:LYS:N	2.80	0.43
1:B:5:PHE:CD2	1:B:76:ARG:HB2	2.53	0.43
1:B:341:VAL:CG1	1:B:342:LYS:H	2.31	0.43
1:B:410:LEU:HG	1:B:458:LEU:HD13	2.00	0.43
1:B:533:VAL:HA	1:B:534:PRO:HD2	1.88	0.43
1:A:230:LEU:C	1:A:232:ASP:H	2.25	0.43
1:B:251:VAL:HG12	1:B:251:VAL:O	2.17	0.43
1:B:260:THR:HG21	1:B:263:LYS:HB2	1.96	0.43
1:B:333:GLY:N	1:B:371:SER:OG	2.51	0.43
1:B:135:ASN:OD1	1:B:136:LYS:N	2.49	0.43
1:B:555:ALA:CB	1:B:557:TYR:CD2	2.99	0.43
1:A:113:GLU:HB3	1:A:114:PRO:CD	2.48	0.43
1:A:267:VAL:O	1:A:270:MET:HG3	2.18	0.43
1:A:434:ASP:OD1	1:A:434:ASP:C	2.61	0.43
1:B:370:TYR:N	1:B:370:TYR:CD1	2.86	0.43
1:A:115:GLN:OE1	1:A:115:GLN:N	2.31	0.43
1:A:202:ASP:OD1	1:A:202:ASP:N	2.51	0.43
1:A:342:LYS:NZ	1:A:394:ASN:O	2.35	0.43
1:A:491:GLN:CG	1:A:512:GLU:HG3	2.48	0.43
1:B:244:ILE:HG13	1:B:244:ILE:H	1.60	0.43
1:A:112:VAL:HG13	1:A:150:THR:CB	2.49	0.43
1:A:505:GLN:N	1:A:575:ASP:CB	2.80	0.43
1:B:9:LYS:HD2	1:B:75:HIS:CD2	2.54	0.43
1:B:574:VAL:CG2	1:B:575:ASP:N	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:LYS:O	1:A:244:ILE:CG1	2.64	0.43
1:A:574:VAL:CG1	1:A:575:ASP:H	2.32	0.43
1:B:646:VAL:HG12	1:B:647:PRO:HD2	2.00	0.43
1:A:140:LEU:O	1:A:142:ALA:N	2.52	0.43
1:A:238:SER:OG	1:A:239:GLU:N	2.50	0.43
1:A:241:LYS:HA	1:A:241:LYS:HD2	1.78	0.42
1:A:270:MET:HG3	1:A:271:LEU:N	2.33	0.42
1:A:510:HIS:HB3	1:A:567:TYR:CE1	2.53	0.42
1:A:579:MET:O	1:A:582:LYS:HB2	2.19	0.42
1:B:355:LEU:HB3	1:B:366:ILE:HG13	2.01	0.42
1:A:201:GLU:OE1	1:A:202:ASP:N	2.46	0.42
1:A:615:TYR:HB3	1:A:618:ASP:OD2	2.18	0.42
1:B:405:GLU:CG	1:B:406:PRO:HD2	2.49	0.42
1:B:412:VAL:HG13	1:B:412:VAL:O	2.18	0.42
1:B:448:VAL:HG22	1:B:449:ILE:N	2.34	0.42
1:B:590:LYS:O	1:B:593:ALA:N	2.52	0.42
1:A:156:GLN:HE21	1:A:637:GLY:HA3	1.84	0.42
1:A:232:ASP:O	1:A:233:GLU:C	2.61	0.42
1:A:290:HIS:HB2	1:A:295:PRO:HA	2.01	0.42
1:A:441:THR:O	1:A:441:THR:HG22	2.19	0.42
1:B:163:GLN:C	1:B:164:LEU:HD12	2.45	0.42
1:B:633:MET:HG2	1:B:634:GLU:N	2.35	0.42
1:A:17:ALA:CB	1:A:105:VAL:HB	2.47	0.42
1:A:549:MET:CE	1:A:559:LEU:HD23	2.48	0.42
1:B:9:LYS:HA	1:B:75:HIS:CD2	2.55	0.42
1:B:670:MET:C	1:B:671:TYR:CD1	2.97	0.42
1:A:469:PHE:N	1:A:469:PHE:HD1	2.16	0.42
1:A:567:TYR:HD1	1:A:568:ASP:HB2	1.83	0.42
1:B:163:GLN:OE1	1:B:175:ILE:HD11	2.19	0.42
1:A:369:VAL:O	1:A:369:VAL:HG12	2.18	0.42
1:A:461:LEU:HD23	1:A:461:LEU:HA	1.83	0.42
1:B:128:VAL:O	1:B:130:ARG:NH2	2.49	0.42
1:B:145:GLU:OE1	1:B:145:GLU:HA	2.20	0.42
1:A:112:VAL:HG13	1:A:150:THR:HB	2.02	0.42
1:A:508:ASP:OD2	1:A:569:GLY:C	2.63	0.42
1:A:614:GLU:OE1	1:A:614:GLU:N	2.48	0.42
1:B:180:GLU:HG3	1:B:182:LYS:HG3	2.01	0.42
1:B:216:GLU:HG3	1:B:229:TYR:CE2	2.55	0.42
1:B:429:LYS:HD3	1:B:429:LYS:HA	1.75	0.42
1:B:90:VAL:CG2	1:B:91:GLU:H	2.20	0.42
1:B:168:ALA:O	1:B:169:GLU:C	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:330:VAL:HG22	1:B:373:ASP:O	2.19	0.42
1:B:590:LYS:HD2	1:B:590:LYS:N	2.34	0.42
1:A:132:VAL:HG21	1:A:151:LEU:HD21	2.02	0.42
1:A:245:ARG:O	1:A:249:THR:OG1	2.25	0.42
1:A:486:PHE:O	1:A:515:PRO:HB3	2.20	0.42
1:A:524:PHE:HE1	1:A:526:ASN:HB2	1.85	0.42
1:A:668:TYR:CD1	1:A:668:TYR:C	2.98	0.42
1:B:133:PHE:CD2	1:B:270:MET:HG3	2.48	0.42
1:A:460:ILE:HD12	1:A:460:ILE:C	2.45	0.41
1:B:32:TYR:CD1	1:B:32:TYR:C	2.98	0.41
1:B:312:LEU:O	1:B:328:PHE:HA	2.20	0.41
1:B:350:GLU:OE1	1:B:382:ASP:HB2	2.20	0.41
1:B:535:ARG:CG	1:B:535:ARG:NH1	2.80	0.41
1:B:579:MET:HG3	1:B:580:ALA:N	2.35	0.41
1:A:235:ILE:HG23	1:A:239:GLU:OE2	2.21	0.41
1:A:237:VAL:O	1:A:240:LEU:HB3	2.20	0.41
1:B:164:LEU:HB2	1:B:176:ILE:CD1	2.42	0.41
1:B:555:ALA:HB1	1:B:557:TYR:CD2	2.54	0.41
1:A:309:PHE:CA	1:A:333:GLY:HA3	2.48	0.41
1:A:162:ILE:HG13	1:A:163:GLN:HG3	2.02	0.41
1:B:164:LEU:HD11	1:B:210:ALA:CB	2.51	0.41
1:B:299:VAL:O	1:B:299:VAL:HG13	2.21	0.41
1:B:335:MET:HE2	1:B:335:MET:HB3	1.92	0.41
1:A:140:LEU:O	1:A:141:GLY:C	2.64	0.41
1:B:278:LEU:CB	1:B:279:PRO:HD2	2.47	0.41
1:B:340:TYR:CD2	1:B:349:ARG:NH2	2.82	0.41
1:B:523:GLU:HB2	1:B:563:LYS:CE	2.44	0.41
1:B:670:MET:HB2	1:B:670:MET:HE3	1.84	0.41
1:A:335:MET:CE	1:A:352:VAL:HG21	2.43	0.41
1:A:528:ILE:HD11	1:A:568:ASP:N	2.35	0.41
1:B:103:VAL:HG22	1:B:131:ILE:CG1	2.51	0.41
1:B:340:TYR:HB3	1:B:392:GLU:OE2	2.21	0.41
1:B:605:MET:SD	1:B:648:LEU:HD13	2.60	0.41
1:A:201:GLU:HA	1:A:204:LEU:CD1	2.50	0.41
1:A:381:LYS:HB2	1:A:381:LYS:HE3	1.90	0.41
1:A:408:ILE:HD11	1:A:478:PRO:CB	2.50	0.41
1:B:483:ARG:HG3	1:B:675:TYR:CE1	2.56	0.41
1:B:554:LEU:HD13	1:B:598:PRO:HG2	2.02	0.41
1:B:688:LYS:C	1:B:690:ASN:H	2.29	0.41
1:A:146:TYR:O	1:A:147:SER:C	2.64	0.41
1:B:410:LEU:HD21	1:B:458:LEU:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:VAL:HG13	1:A:150:THR:OG1	2.20	0.40
1:B:569:GLY:O	1:B:570:SER:HB3	2.21	0.40
1:B:670:MET:O	1:B:671:TYR:HD1	2.05	0.40
1:B:619:ILE:O	1:B:622:ASP:HB3	2.21	0.40
1:A:567:TYR:CD1	1:A:567:TYR:C	2.99	0.40
1:B:17:ALA:CB	1:B:23:LYS:HB2	2.51	0.40
1:B:330:VAL:HG23	1:B:330:VAL:O	2.21	0.40
1:B:466:LYS:O	1:B:470:ASN:HA	2.21	0.40
1:A:80:ILE:HG12	1:A:98:VAL:CG1	2.52	0.40
1:A:115:GLN:CD	1:A:115:GLN:N	2.75	0.40
1:A:297:GLU:CD	1:A:297:GLU:N	2.77	0.40
1:B:138:ASP:OD2	1:B:263:LYS:HG3	2.21	0.40
1:B:415:LYS:HZ2	1:B:474:ASN:N	2.19	0.40
1:B:512:GLU:HG2	1:B:565:LYS:HB3	2.03	0.40
1:B:659:ARG:O	1:B:660:SER:C	2.63	0.40
1:A:6:SER:O	1:A:7:LEU:C	2.63	0.40
1:A:399:GLU:CG	1:A:400:SER:N	2.85	0.40
1:B:219:ALA:HA	1:B:225:LEU:CD1	2.43	0.40
1:B:487:LYS:HE2	1:B:599:VAL:HG13	2.03	0.40
1:B:688:LYS:HA	1:B:691:LYS:NZ	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	639/693 (92%)	593 (93%)	44 (7%)	2 (0%)	36	67
1	B	639/693 (92%)	580 (91%)	58 (9%)	1 (0%)	43	73
All	All	1278/1386 (92%)	1173 (92%)	102 (8%)	3 (0%)	43	73

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	362	SER
1	A	360	ALA
1	B	251	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	543/579 (94%)	489 (90%)	54 (10%)	7	28
1	B	543/579 (94%)	490 (90%)	53 (10%)	7	28
All	All	1086/1158 (94%)	979 (90%)	107 (10%)	7	28

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	THR
1	A	34	THR
1	A	112	VAL
1	A	140	LEU
1	A	154	ARG
1	A	179	VAL
1	A	192	THR
1	A	199	ILE
1	A	201	GLU
1	A	213	SER
1	A	218	VAL
1	A	227	GLU
1	A	230	LEU
1	A	234	GLU
1	A	236	SER
1	A	244	ILE
1	A	246	GLN
1	A	270	MET
1	A	304	ASP
1	A	309	PHE
1	A	330	VAL

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Mol	Chain	Res	Type
1	A	344	SER
1	A	361	ASN
1	A	368	THR
1	A	369	VAL
1	A	380	LEU
1	A	396	ILE
1	A	400	SER
1	A	411	SER
1	A	447	GLN
1	A	448	VAL
1	A	450	ILE
1	A	459	ASP
1	A	462	VAL
1	A	463	ASP
1	A	495	LYS
1	A	505	GLN
1	A	509	VAL
1	A	514	THR
1	A	518	THR
1	A	533	VAL
1	A	536	GLU
1	A	571	TYR
1	A	578	GLU
1	A	611	MET
1	A	618	ASP
1	A	630	VAL
1	A	631	ASP
1	A	634	GLU
1	A	640	GLN
1	A	649	SER
1	A	667	THR
1	A	671	TYR
1	A	685	ASP
1	B	29	ARG
1	B	88	LEU
1	B	92	VAL
1	B	109	GLN
1	B	112	VAL
1	B	118	THR
1	B	122	GLN
1	B	162	ILE
1	B	175	ILE

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Mol	Chain	Res	Type
1	B	176	ILE
1	B	178	LEU
1	B	187	THR
1	B	192	THR
1	B	201	GLU
1	B	225	LEU
1	B	230	LEU
1	B	235	ILE
1	B	238	SER
1	B	246	GLN
1	B	264	ASN
1	B	271	LEU
1	B	280	SER
1	B	288	ILE
1	B	293	SER
1	B	318	THR
1	B	336	THR
1	B	363	ARG
1	B	369	VAL
1	B	397	ILE
1	B	420	GLN
1	B	425	GLN
1	B	436	THR
1	B	442	ASP
1	B	475	VAL
1	B	528	ILE
1	B	532	VAL
1	B	536	GLU
1	B	547	ASP
1	B	550	GLU
1	B	574	VAL
1	B	579	MET
1	B	611	MET
1	B	618	ASP
1	B	622	ASP
1	B	624	THR
1	B	625	SER
1	B	629	ARG
1	B	636	ARG
1	B	641	VAL
1	B	646	VAL
1	B	659	ARG

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Mol	Chain	Res	Type
1	B	667	THR
1	B	688	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	143	ASN
1	A	156	GLN
1	A	246	GLN
1	A	409	HIS
1	A	505	GLN
1	A	572	HIS
1	A	690	ASN
1	B	18	HIS
1	B	75	HIS
1	B	115	GLN
1	B	143	ASN
1	B	264	ASN
1	B	431	GLN
1	B	447	GLN
1	B	551	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	649/693 (93%)	-0.20	4 (0%)	85 72	55, 104, 163, 250	0
1	B	649/693 (93%)	-0.11	3 (0%)	87 75	68, 115, 175, 278	0
All	All	1298/1386 (93%)	-0.15	7 (0%)	87 75	55, 109, 168, 278	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	10	THR	2.5
1	A	581	PHE	2.4
1	B	637	GLY	2.3
1	B	391	GLY	2.1
1	A	372	GLY	2.1
1	A	666	GLY	2.0
1	B	253	PHE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.